

Lau, Berciu and Sawatzky reply: In the preceding Comment[1], Lee and Lee bring to attention their interesting variational calculation for the single band Hubbard model further reduced to a t - t' - t'' - J model [2]. Its main result was to reveal new low-energy one-hole states called spin-bags (SB), possibly forming a continuum. SBs consist of a quasiparticle (QP) plus a spin-wave excited in the AFM background, and are found to cross below the QP band in some regions of the Brillouin zone (BZ). Based on this, Lee and Lee claim that the SBs explain, within a one-band model, the spin- $\frac{3}{2}$ polaron that we recently found in a three-band model [3]. They conclude that our claim that this model reveals physics that cannot be described within one-band models, *i.e.* in the framework of Zhang-Rice singlets (ZRS), is not justified.

While superficial similarities exist between the SB and the spin- $\frac{3}{2}$ polaron, we disagree that they describe the same physics, on several grounds:

(i) In the Supplemental Material of Ref. [3], we ruled out the possibility that the spin- $\frac{3}{2}$ polaron is a spin- $\frac{1}{2}$ polaron plus a free magnon, because its band lies below the continuum describing such states. It can be roughly thought of as a bound-state of a spin- $\frac{1}{2}$ polaron and a magnon, with a very distinct local spin structure around the charge. The existence of such bound states, which might be a better analog of our spin- $\frac{3}{2}$ polaron, is not analyzed for the one-band model, in Refs. [1, 2];

(ii) As shown in our Fig. 2, the spin- $\frac{3}{2}$ polaron's band has significant dispersion, comparable to that of the spin- $\frac{1}{2}$ polaron [3]. In contrast, the low-energy edge of the SB continuum is rather flat throughout the BZ, see Fig. 1(b) of Ref. [2]. This striking difference in their spectra is likely an indication of a very different nature of the two types of low-energy states. There is currently no evidence that the two models have comparable dispersion for spin excitations, regardless of their nature.

(iii) While the spin- $\frac{3}{2}$ polaron band crosses below the spin- $\frac{1}{2}$ polaron band in certain regions, just like the SB continuum is below the QP band in certain regions of the BZ, a careful comparison shows yet more differences. In our model, this happens in two separate regions, centered at $(0,0)$ and (π,π) . In the variational solution for the one-band model, this happens in one larger region centered at $k = (\pi,\pi)$ which, coincidentally, is the AFM order vector. The difference is most clearly visible along the $(\pi,0) - (0,\pi)$ cut, where we find no crossing whereas the variational calculation predicts the QP as the low-energy state only near $(\frac{\pi}{2}, \frac{\pi}{2})$. If bound-states were found in the one-band model, the comparison would be worse since this would further increase the crossing region.

Such differences result in very different physics, *eg.* at the nodal point. While the vanishing quasiparticle weight at $(0,\pi)$ is explained as being due to the SB state in the one-band model, we find $Z = 0$ here because of the orthogonal reflection parity between the lowest electron-removal state and the lowest spin- $\frac{1}{2}$ eigenstate [4].

A second point raised in the Comment is that if a ZR-like state is built from a superposition of configurations like that of Fig. 3a, AFM correlations on the e and d bonds are similar to those calculated in Ref. [2]. This is taken as proof that the spin- $\frac{1}{2}$ polaron is similar to the ZR-based QP state, as well. First, Fig. 3a is for a state of momentum $(\frac{\pi}{2}, \frac{\pi}{2})$, so naive $\frac{\pi}{2}$ rotations lead to a state with an ill defined momentum. In fact, even though these bonds are related by the exact $\hat{P}_{x \leftrightarrow y}$ symmetry of our Hamiltonian, the quoted values are not equal; this is wrong. In any case, the fact that bonds rather far from the hole show robust AFM correlations is hardly surprising. The key observation in our model is the strong FM correlation between the spins neighboring the hole, which points to the three-spin polaron (3SP) as the proper framework to understand the spin- $\frac{1}{2}$ polaron and the inner core of the spin- $\frac{3}{2}$ polaron. Since the 3SP can be written as the sum of singlets between the hole and each of its neighboring spins [3], it does have a finite overlap with a ZR state [5]. Its additional degrees of freedom, however, allow it to describe correlations beyond those possible in a ZR-based model. This invalidates the Comment's claim that a low-energy non-bonding state is the only signature of breakdown for a one-band model. It is very important, in this context, to also point out that the model used in Ref. [2] is a further simplification of the ZR scenario – the O states are no longer present and a discussion of the spin correlations around an O hole becomes meaningless.

For all these reason we remain convinced that both the spin- $\frac{1}{2}$ and spin- $\frac{3}{2}$ polarons in our 3 band model are quite different objects from the QP and SB obtained from a single band description. However, caution is necessary since comparisons between a variational solution based on mean-field and our exact diagonalization (ED) for a finite cluster may be misleading. If ED results for a one-band model revealed similar low-energy spin- $\frac{3}{2}$ states, and FM correlations between the spins sandwiching the hole, our position would have to be reconsidered. To our knowledge, the former is not the case and the latter is not possible for a one-band model.

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- [1] W.-C. Lee and T. K. Lee, preceding Comment (arXiv:1108.5413v1).
 - [2] W.-C. Lee, T. K. Lee, C.-M. Ho, and P. W. Leung. Phys. Rev. Lett. **91**, 057001 (2003).
 - [3] B. Lau, M. Berciu, and G. A. Sawatzky. Phys. Rev. Lett. **106**, 036401 (2011).
 - [4] B. Lau, M. Berciu, and G. A. Sawatzky, arXiv:1107.4141
 - [5] See, for example, Ref. [18] in our Letter.